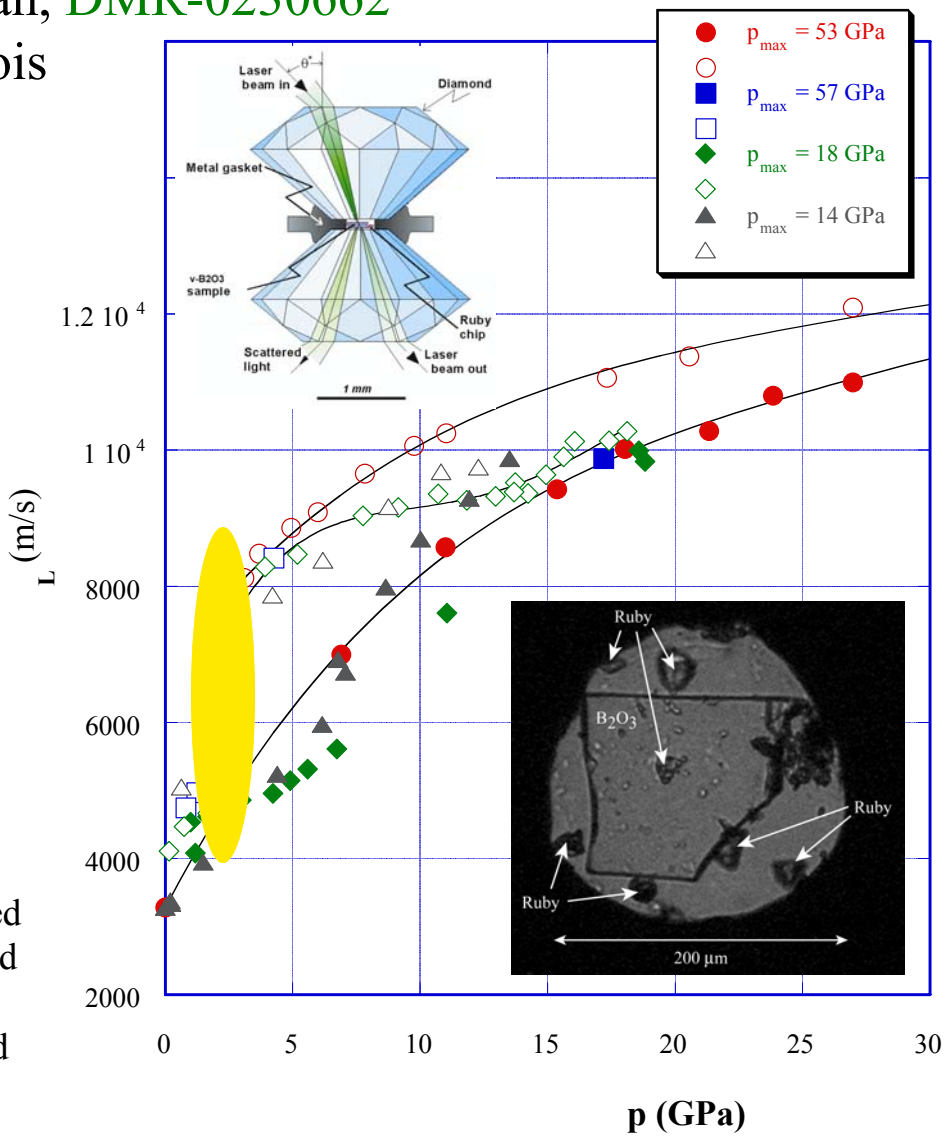
Polyamorphism and Structural Transitions during Glass Formation

John Kieffer, PI, University of Michigan, DMR-0230662
Jay D. Bass, Co-PI, University of Illinois

Polyamorphism, i.e., the existence of two distinct non-crystalline states for the same material, has been evidenced for vitreous B_2O_3. The pressure-induced transformation between low-density (BO_3-units) and high-density (BO_4-units) B_2O_3 is continuous upon compression and 1st-order upon de-compression, as revealed by the change in sound velocity.



High-pressure Brillouin scattering experiments are carried out using a diamond anvil cell. The specimen in enclosed between flattened diamond tips by a metal gasket. The diamonds allow for the application of high pressures and act as windows for the probing radiation.

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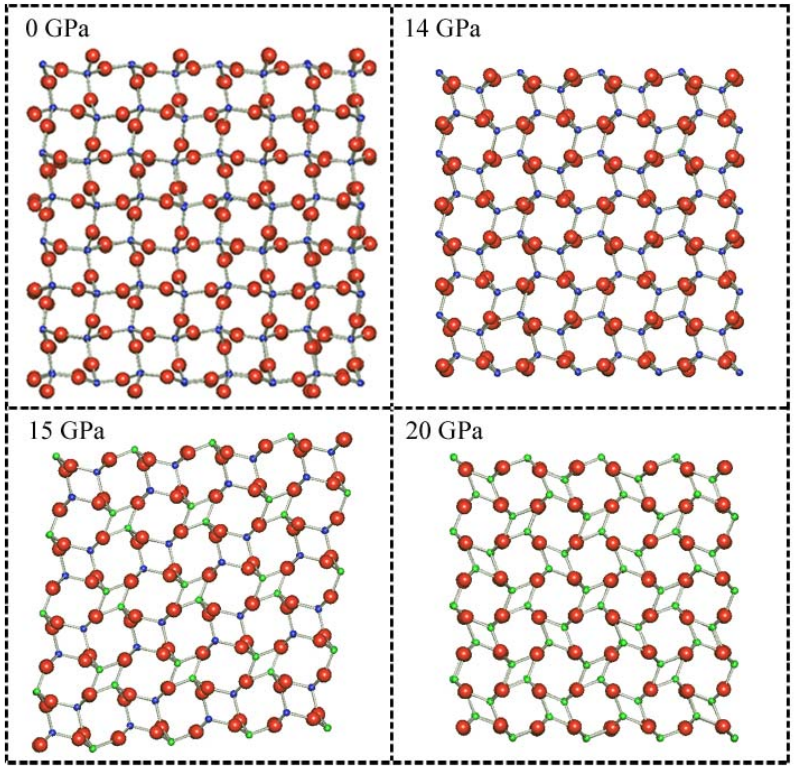
A structural transition to a new high-density form of cristobalite is observed in our molecular dynamics simulations (both classical and *ab inito*). The transformation mechanism involves a two-step shearing process and results in a structure where oxygen is arranged in a simple cubic sublattice. The resulting structure has never been reported, but the corresponding x-ray diffraction pattern matches that of an experimentally observed high-density silica phase that so far remained unidentified.



The structure at 0 GPa is α-cristobalite. The transformation takes place between 14 and 16 GPa, and involves a transient sheared state.

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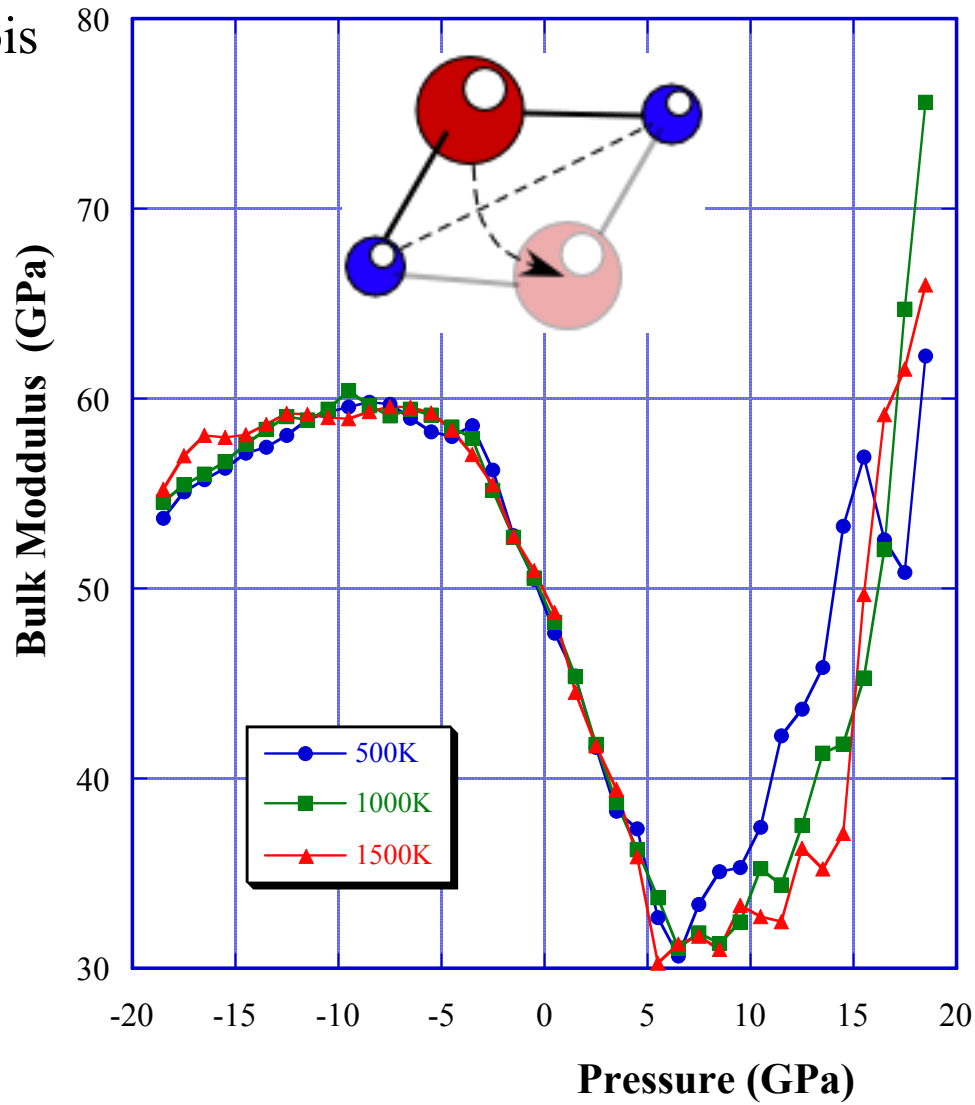
Molecular dynamics simulations of silica glass reveals that the anomalous decrease of the elastic modulus with increasing pressure is due to abrupt and localized structural transitions, involving the rotation of Si-O-Si units about the Si-Si axis, similar to the mechanism underlying the α-to-β transformation in cristobalite.

A similar mechanism is responsible for the positive temperature dependence of the elastic modulus.



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Education:

Three undergraduate (Ranjeet Rao, Surair Bashir, Vashist Vasanthakumar) and two graduate students (Liping Huang and Jason Nicholas) contributed to this work. Ranjeet is now a graduate student at the University of Illinois and recipient of an NSF Graduate Fellowship. Surair (an African-American female) and Vashist are undergraduates at Michigan and still involved in the project. Jason has graduated with an M.S. degree in May '03, and is now a Ph.D. student at U.C. Berkeley. Liping is expected to receive her Ph.D. in '04. She has won the 2003 Norbert J. Kreidl Award from the American Ceramic Society for work on this subject.

Outreach:

The PI is co-organizer and participant in the Materials Camp held annually at Michigan. 20 high school science teachers spend a week learning about materials science, with the goal of using this information in their curricula and teach high school students about the role of materials in technology.